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Microscopic phenomenon in light of classical and quantum theory

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Abstract : Quantum mechanical boundary corrected continuum intermediate state (BCCIS) approximation and classical trajectory Monte Carlo (CTMC) simulation method have been employed to study total charge transfer cross sections in collisions of Be^{q+} (q = 2–4) and B^{q+} (q = 3–5) with atomic hydrogen in ground state in the energy range of 30 - 200 keV/amu Results have been found to be in reasonable agreement with each other Attempts have been made to find justifications for such resemblance

Keywords . Heavy ion-atom collisions, charge transfer, cross sections

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1. Introduction

Let us consider the bound motion of a particle (A) in the field of an another particle (B). Let the force between them obeys inverse square law, $F_{AB} = \frac{k}{r^2}$, where constant k is determined by nature of interaction *i.e.* gravitational or coulombic. If we solve the problem in framework of classical mechanics, all properties of motion are predicted quite accurately, if A and B happen to be celestial bodies. If B and A are proton and electron respectively, it is a standard textbook exercise to show that binding energy comes out as [1]

$E = -\frac{2\pi^2\mu Z^2 e^4}{J^2}$, where J is related to some action variable which is continuous in nature and other symbols have usual meanings. If we solve the same problem in the framework of quantum mechanics, binding energy expression is found as [2]

$$E = -\frac{2\pi^2\mu Z^2 e^4}{n^2 h^2}.$$

In this case, we find discrete spectrum which reproduces experimental observations where classical mechanics fails. There are such numerous observations *viz* tunneling, spin *etc.* which can not be explained by the tools of classical mechanics. So physical events may be termed either as macroscopic or as microscopic. Unique classification of physical events as macroscopic or microscopic is a formidable task. However, they may be classified grossly in terms of length and energy scale. With this sense in mind, the collisions of heavy ions with atoms may be termed as microscopic events. Does it mean that we can not apply laws of classical mechanics to find out the properties of heavy ion-atom collision ?

This lecture is motivated to address such queries. If we look through the results of findings [3] of classical limit of quantum mechanical formalisms, we may find the following interpretations : (i) Ensemble interpretation (EI), (ii) Single particle interpretation (SPI) and (iii) Inconclusive. Now, if we accept EI as one of the meaningful results, we may expect satisfactory results for heavy ion-atom interaction when we project classical equations of motion in an ensemble environment. Practically, this may be the basic theme underlying classical trajectory Monte Carlo simulation (CTMC) method applied to ion-atom collisions.

We shall now formulate the problem of heavy ion-atm collisions in the framework of both classical and quantum mechanics and results will be discussed in the cases of collisions of different degree ions of Be and B with ground state atomic hydrogen. These systems have been chosen due to the fact that Be and B have been identified as the plasma facing materials in the design of modern fusion reactors [4].

2. Theoretical formulation

Collision diagram is shown in Figure 1. Let a, b, μ_T and μ_P are reduced masses related to co-ordinates r_{Te}, r_{Pe}, R_T and R_P respectively.

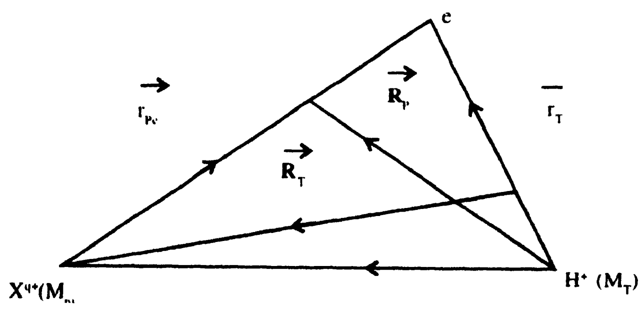

Figure 1 Coordinate representation for the reaction X^{q+} ($Be^{(2-4)+}$ or $B^{(1-5)+}$) + $H(1s) \rightarrow X^{(q-1)+}$ (nl) + H^+

(i) Classical formalism :

Theoretical formalism of collision event in the framework of classical mechanics develops step by step in an analogous manner to those of experimental procedure for the same investigation. Such one to one correspondence between theory and experiment may be shown as follows.

Experiment		Theory	
(i)	Preparation of initial system	(i)	Initialisation
(ii)	Collision	(ii)	Step by step integration of classical equations of motion
(iii)	Detection	(iii)	Exit test and determination of cross section

Classical Hamiltonian of the whole system may be written as

$$H = \frac{1}{2a}\left(p_1^2 + p_2^2 + p_3^2\right) + \frac{1}{2\mu_T}\left(p_4^2 + p_5^2 + p_6^2\right)$$

$$+ V_{Te}(\boldsymbol{r}_{Te}) + V_{pe}(\boldsymbol{r}_{pe}) + V_{Tp}(\boldsymbol{R}), \tag{1}$$

where $r_{pe}^2 = (aq_1 - q_4)^2 + (aq_2 - q_5)^2 + (aq_3 - q_6)^2$

$$r_{Te}^2 = q_1^2 + q_2^2 + q_3^2 . \tag{2}$$

Here q_i, p_i (i = 1, 3) be the rectangular coordinates and conjugate momenta of the electron relative to the centre of mass of the target system. The corresponding quantities of the projectile are q_i, p_i (i = 4 – 6) respectively in the centre of mass system.

Hamilton's equation of motion may be written as

$$p_i = a\dot{q}_i \qquad i = 1, 2, 3,$$

$$p_i = \mu_T q_i \qquad i = 4, 5, 6, \tag{3}$$

and

$$\dot{p}_i = -\frac{1}{r_{pe}}\frac{\partial V}{\partial r_{pe}}a(aq_i - q_{i+3}) - \frac{1}{r_{Te}}\frac{\partial V}{\partial r_{Te}}q_i$$

$$-\frac{1}{R}\frac{\partial V}{\partial R}\frac{a}{\mu_T}\left(\frac{a}{\mu_T}q_i + q_{i+3}\right), \quad i = 1, 2, 3, \tag{4}$$

$$\dot{p}_i = -\frac{1}{r_{pe}}\frac{\partial V}{\partial r_{pe}}(q_i - aq_{i-3}) - \frac{1}{R}\frac{\partial V}{\partial R}\left(q_i + \frac{a}{\mu_T}q_{i-3}\right) \quad i = 4, 5, 6$$

where $V = V_{Te}(\boldsymbol{r}_{Te}) + V_{pe}(\boldsymbol{r}_{pe}) + V_{Tp}(\boldsymbol{R})$.

These twelve equations in two sets given by eqs. (3) and (4) completely describe the motion of the whole system in centre of mass coordinates.

These coupled equations are integrated numerically step by step from $t = -\infty$ to $t = +\infty$. At $t = -\infty$, the target system is unperturbed. So initial values for q_i and p_i (i = 1, 6) may be assigned in terms of six random numbers [5] from a sequence of random numbers. At $t = +\infty$, q_i and p_i (i = 1, 3) are determined. From these values of q_i and p_i (i = 1, 3), energies (E_{Te} and E_{pe}) of the electron in the sub-systems *i.e.* (electron, target) and (electron, projectile) respectively are determined. Then the processes are distinguished as

(a) Charge transfer, $E_{pe} < 0$, $E_{Te} > 0$

(b) direct ionization, $E_{pe} > 0$, $E_{Te} > 0$, $r_{Te} < r_{pe}$ (5)

(e) transfer ionization, $E_{pe} > 0$, $E_{Te} > 0$, $r_{Te} > r_{pe}$

(d) elastic scattering and direct excitation, $E_{pe} > 0$, $E_{Te} < 0$.

Total ionization comes from the sum of direct and transfer ionization. Calculations are repeated . for several thousand trajectories.

If N_T is the total number of trajectories calculated and $N_{R'}$ number of trajectories satisfies any of the criteria for a specific reaction (a) – (d), the cross sections are given by

$$\sigma_R = (N_R / N_T)\, \pi b_{max}^2 , \tag{6}$$

where b_{max} is the maximum impact parameter beyond which no reaction takes place. The standard error is estimated in either of the following ways.

$$S^2 = \sigma_R \left(\frac{\pi b_{max}^2 - \sigma_R}{N_T - 1} \right),$$

$$S^2 = \sigma_R \frac{(N_T - N_R)}{N_T N_R} . \tag{7}$$

(ii) Quantum mechanical formalism :

Quantum mechanical Hamiltonian of the whole system may be written as

$$H = H_0 + V_{Te}(r_{Te}) + V_{Pe}(r_{Pe}) + V_{TP}(\boldsymbol{R}), \tag{8}$$

where $\quad H_0 = -\frac{1}{2\mu_T} \nabla_{R_i}^2 - \frac{1}{2a} \nabla_{r_{Te}}^2$ (entrance channel)

$$= -\frac{1}{2\mu_p} \nabla_{R_p}^2 - \frac{1}{2b} \nabla_{r_{pe}}^2 \text{ (exit channel).} \tag{9}$$

In case of charge transfer, channel hamiltonians may be written as

$$H = \underbrace{-\frac{1}{2\mu_T} \nabla_{R_i}^2 - \frac{1}{2a} \nabla_{r_{Te}}^2 + V_{Te}(\boldsymbol{r}_{Te})}_{H_i} + \underbrace{V_{Pe}(\boldsymbol{r}_{Pe}) + V_{TP}(\boldsymbol{R})}_{V_i} \tag{10}$$

$$= \underbrace{-\frac{1}{2\mu_P} \nabla_{R_p}^2 - \frac{1}{2b} \nabla_{r_{pe}}^2 + V_{Pe}(\boldsymbol{r}_{Pe})}_{H_f} + \underbrace{V_{Te}(\boldsymbol{r}_{Te}) + V_{Tp}(\boldsymbol{R})}_{V_f}$$

and the corresponding channel wave functions may be written as

$$(E - H_i)\psi_i = 0, \ (E - H_f)\psi_f = 0, \tag{11}$$

where $\quad \psi_i = \Phi_i(\boldsymbol{r}_{Te})\, e^{i\boldsymbol{k}_i \cdot \boldsymbol{R}_i}, \ \psi_f = \Phi_f(\boldsymbol{r}_{Pe})\, e^{i\boldsymbol{k}_f \cdot \boldsymbol{R}_p}$

and

$$E = \frac{K_i^2}{2\mu_T} + \varepsilon_i \text{ (entrance channel)}$$

$$= \frac{K_f^2}{2\mu_P} + \varepsilon_f \text{ (exit channel)} \tag{12}$$

where $\phi_i\,(\phi_f)$, $E_i\,(E_f)$ and $K_i\,(K_f)$ are respectively initial (final) bound-state wave function, initial (final) binding energy and initial (final) momentum of relative motion of colliding system

The prior form of the transition amplitude (with the first term only) in the formalism of Dodd and Greider [6] may be written in the framework of distorted wave theory as

$$T_{if}^{(\ )} = \left\langle \psi_f \middle| \omega_f^{-*} \left[1 + g_x^{-} (V_f - W_f)\right]^* (V_i - W_i)\, \omega_i^{+} \middle| \psi_i \right\rangle, \tag{13}$$

where Moller operators ω_i^+, ω_f^- and g_x^- are defined as

$$\omega_i^+ = 1 + \frac{1}{E - H_i - W_i + i\eta} W_i,$$

$$\omega_f^- = 1 + \frac{1}{E - H_f - W_f - i\eta} W_f, \tag{14}$$

$$g_x^- = \frac{1}{E - H + V_x - i\eta},$$

where $W_i\,(W_f)$ is the distorting potential in initial (final) channel and V_x is a distorting potential in an intermediate channel whose choice is restricted by the condition that it should contain no two-body potential occurring in V_i.

Now if we substitute

$$\omega_f^- \left| \psi_f \right\rangle = \left| \chi_f^- \right\rangle$$

and $$\left[1 + g_x^- (V_f - W_f)\right] \left| \chi_f^- \right\rangle = \left| \xi_f^- \right\rangle \tag{15}$$

then $\left| \xi_f^- \right\rangle$ satisfies the equation (in the limit $\eta \to 0$)

$$(E - H + V_x) \left| \xi_f^- \right\rangle = 0, \tag{16}$$

provided that $V_x \left| \chi_f^- \right\rangle = 0$.

Now writing $\left|\xi_f^-\right\rangle = \left|\phi_f(r_{Pe})\, g_f^-\right\rangle$ and substituting in eq. (16), we may find

$$\phi_f(r_{Pe})\left[E-\varepsilon_f - H_0 - V_{Tp}(\boldsymbol{R}) - V_{Te}(\boldsymbol{r}_{Te})\right]G_f^-$$

$$+\frac{1}{b}\nabla_{r_{Pe}}\phi_f(r_{Pe}).\nabla_{r_{Pe}}G_f^- + V_i\,\xi_f^- = 0. \tag{17}$$

Choosing $V_i\,\xi_f^- = -\frac{1}{b}\nabla_{r_{Pe}}\phi_f(r_{Pe}).\nabla_{r_{Pe}}G_f$

and on substitution in eq (17), we may find that G_f^- satisfies the differential eq.

$$\frac{K_f^2}{2\mu_P}+\frac{1}{2\mu_T}\nabla^2_{R_f}+\frac{1}{2a}\nabla^2_{r_{Te}}+V_{Te}(\boldsymbol{r}_{Te})+V_{TP}(\boldsymbol{R}_f)\;\; G_f^- = 0. \tag{18}$$

Now, if $V_{Te}(r_{Te})$ and $V_{Tp}(\boldsymbol{R})$ happen to be coulomb potential, the exact solution for G_f^- [7] may be found out. Now, the transition amplitude may be written accordingly and cross sections may be computed easily. The essence of this method lies in the fact that it takes into account of the intermediate states of the target and proper boundary condition is satisfied.

3. Results and discussion

Results computed from quantum mechanical BCCIS-method [7] and classical CTMC-method [5] are displayed in Figures 2-7 in case of interactions of ground state atomic hydrogen with Be^{2+}, Be^{3+}, Be^{4+}, B^{3+}, B^{4+} and B^{5+} respectively. The interaction of the active electron with the projectile ion has been treated in different ways. The projectile ion has been treated as a rigid core ion due to screening by passive electrons and the charge (Z_p) on the projectile ion is

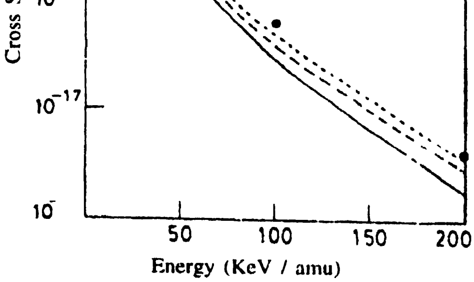

Figure 2. Total capture cross sections for Be^{2+}+ H(1s) collisions Theory —, present work (model potential), ..., present work (SS-model), - - -, present work (BES-model), and ● ● ● CTMC results [13, 14]

determined by (i) binding energy screening [8, 9] (BES) *i.e.* $Z_p = (-2\eta_f^2 \varepsilon_f)^{1/2}$ where ε_f is the binding energy of the electron in the final state represented by principal quantum number n_f; and (ii) slater screening [8,9] (SS), *i.e.* $Z_p = Z - \delta$ where Z is the nuclear charge of the projectile

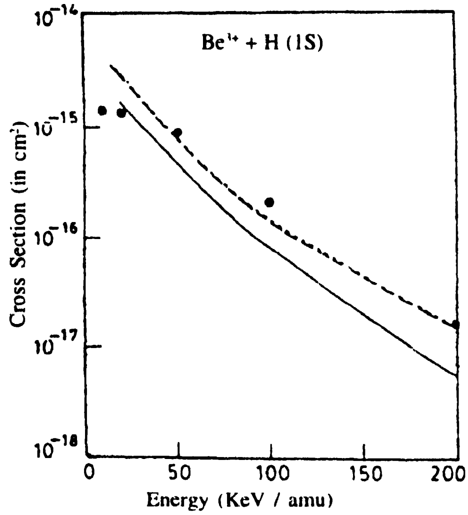

Figure 3. Same as Figure 2

and δ [10] is the total screening charge by the passive electrons. In these two cases, the final state wavefunction is hydrogenic with effective number charge Z_p. (iii) In other case, the interaction of the active electron with the projectile ion has been estimated by a model potential as

$$V_{Pe}(r_{Pe}) = -\frac{q}{r_{Pe}} - \frac{e^{-\lambda r_{Pe}}}{r_{Pe}}\left[(Z-q)+br_{Pe}\right]$$

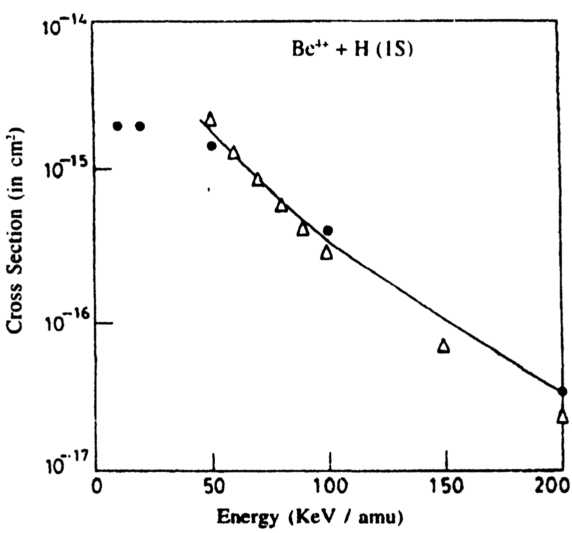

Figure 4. Total capture cross sections for Be^{4+} + $H(1s)$ collisions. Theory : ——, present work ; ΔΔΔ the results of CDW-EFS method of Busengo *et al* [15] and ●●●, CTMC results [13, 14].

where Z and q are respectively the nuclear and asymptotic charge of the projectile ion. b and λ are two arbitrary parameters chosen variationally with respect to a slater basis set in such a way that corresponding Hamiltonian of the active electron in the final state is diagonalised to reproduce correct energies. Model potential parameters are given in tabular form in our earlier work [11].

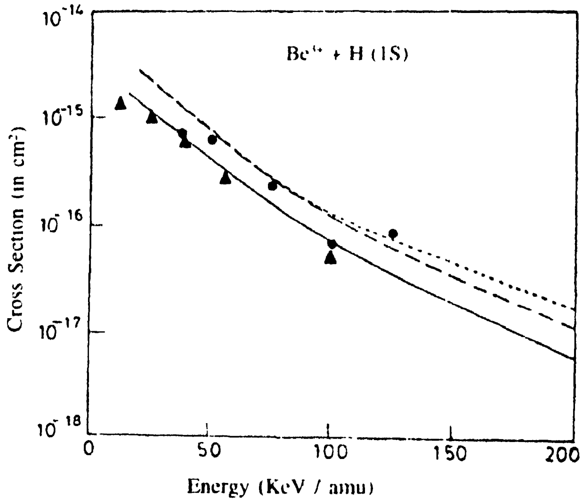

Figure 5. Total capture cross sections for B^{4+} + $H(1s)$ collisions. Theory ——, present work ; (model potential), ... , present work (SS-model), - - -, present work (BES-model), ▲, the results of Hansen and Dubois [16] and ●, CTMC results [14, 17]

From Figure 2, we find that variation of total cross sections with impact energies in case of Be^{2+} + H interaction has fair agreement between two sets of results. In case of collisions of Be^{3+} with atomic hydrogen, agreement are more closer (shown in Figure 3) except for the results obtained from model potential approach. For Be^{4+} + H collision, experimental results

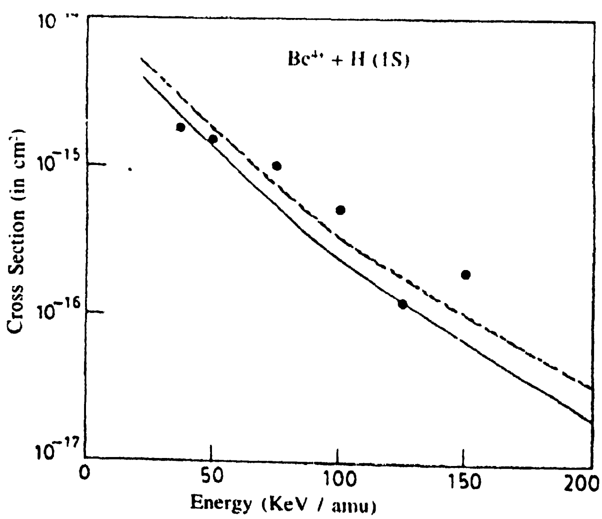

Figure 6. Total capture cross sections for B^{4+} + $H(1s)$ collisions. Theory : ——, present work ; (model potential), ... , present work (SS-model), - - - - - - - -, present work (BES-model, and ● ● ●, CTMC results [5, 14]

[12], CTMC results [13, 14] and BCCIS-results [11] have excellent agreement (shown in Figure 4). In case of collisions of $B^{q+}(q = 3-5)$ with atomic hydrogen (shown in Figure 5-7), classical and quantum mechanical results have more or less satisfactory agreement.

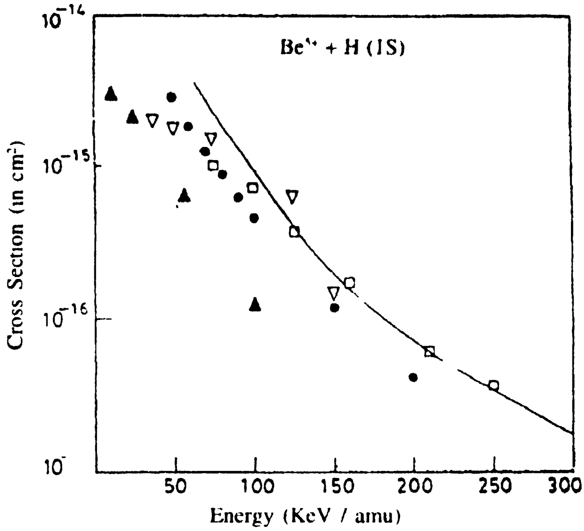

Figure 7. Total capture cross sections for B^{4+} + $H(1s)$ collisions Theory — —, present theory, ▽▽▽ CTMC results [5, 14] ▲▲▲, results of Hansen and Dubois [16], ●●●, results of Busnengo *et al* [15] Expt □□□, results of Goffe *et al* [12]

4. Concluding remarks

Calculated quantum mechanical results are exhaustive and rigorous. On the other hand, classical results have been obtained from several thousand trajectories. Agreement between these two sets of results in case of heavy ion-atom collisions indicate that ensemble interpretation could be well accepted in determining the classical limit of quantum mechanical formulation.

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